



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:43 am BST

PDB ID : 3I7P
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR40A
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Deposited on : 2009-07-08
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

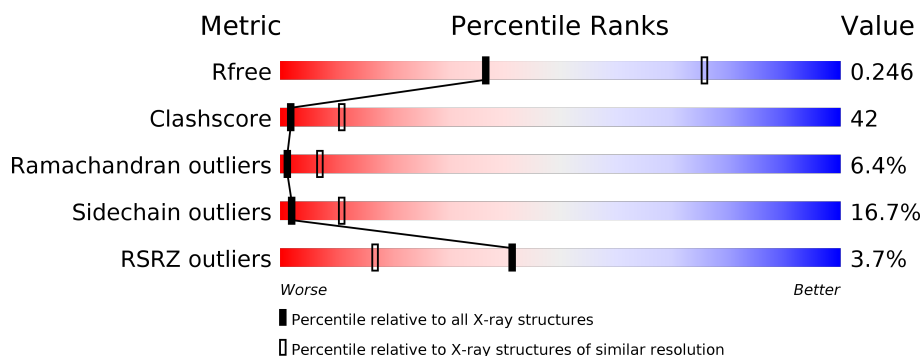
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1143	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>42%</div> <div>13%</div> <div>..</div> </div> </div>
2	B	13	<div> <div>15%</div> <div> <div></div> <div>69%</div> <div>31%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8842 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1114	Total	C	N	O	S	0	0	0
			8726	5529	1472	1677	48			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	SER	-	EXPRESSION TAG	UNP Q16531
A	0	HIS	-	EXPRESSION TAG	UNP Q16531
A	422	TYR	ASP	SEE REMARK 999	UNP Q16531
A	898	ASP	GLU	SEE REMARK 999	UNP Q16531
A	899	VAL	LEU	SEE REMARK 999	UNP Q16531

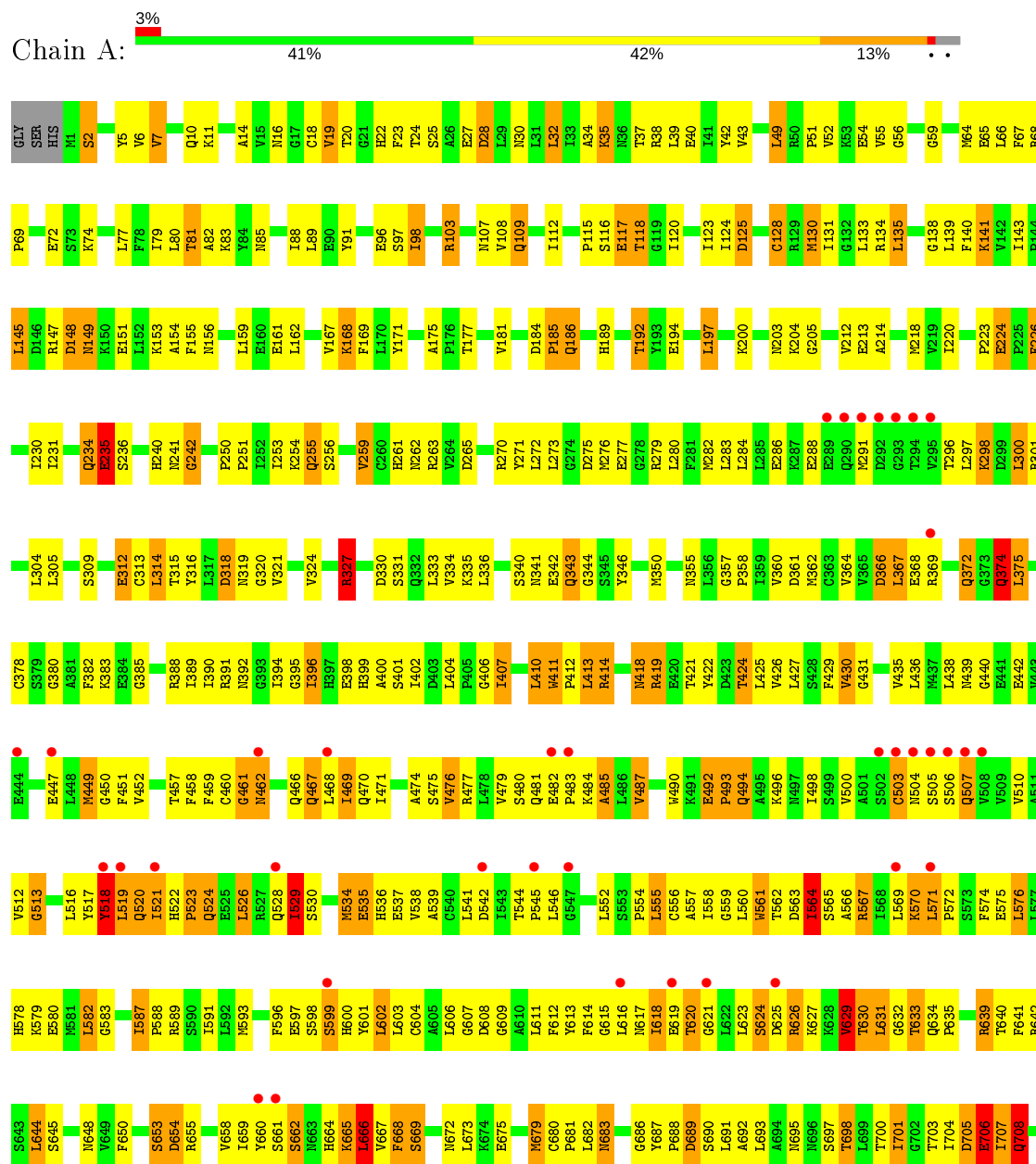
- Molecule 2 is a protein called WD repeat-containing protein 40A.

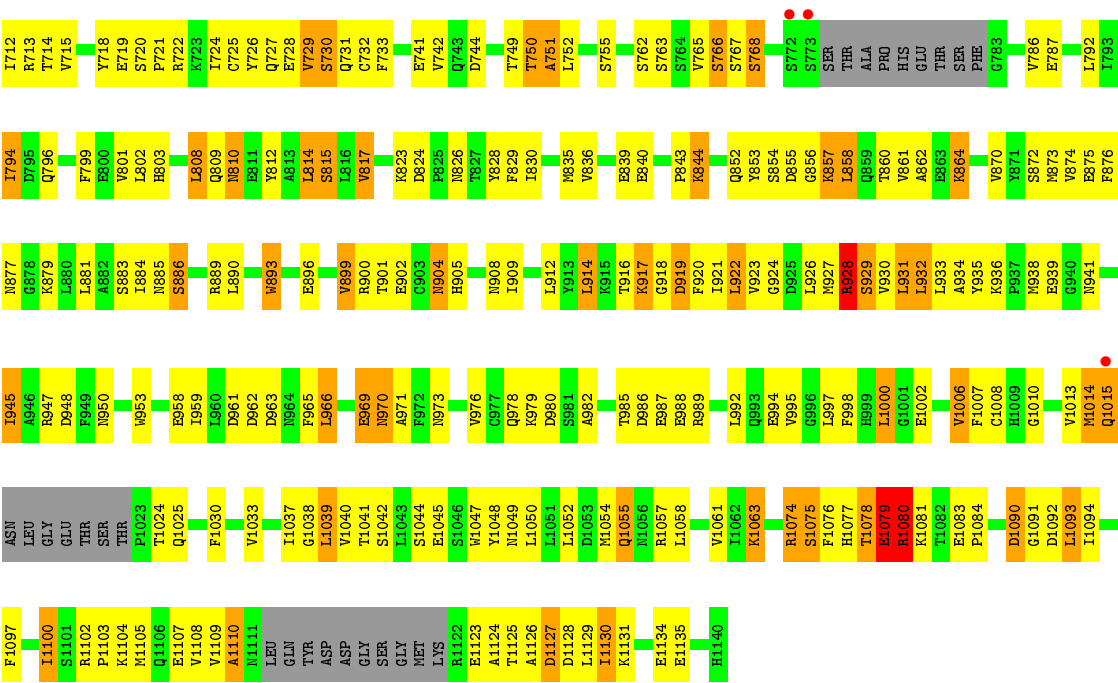
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	76	21	19			

3 Residue-property plots

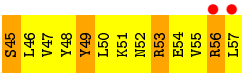
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA damage-binding protein 1





● Molecule 2: WD repeat-containing protein 40A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 132.52Å 183.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 3.00 44.89 – 2.98	Depositor EDS
% Data completeness (in resolution range)	87.0 (45.79-3.00) 86.7 (44.89-2.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.301 0.251 , 0.246	Depositor DCC
R_{free} test set	1410 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8842	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	5/8885 (0.1%)	0.95	27/12034 (0.2%)
2	B	1.16	0/117	0.91	0/156
All	All	0.81	5/9002 (0.1%)	0.95	27/12190 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	CYS	CB-SG	-10.32	1.64	1.82
1	A	1008	CYS	CB-SG	-8.48	1.67	1.82
1	A	924	GLY	N-CA	5.49	1.54	1.46
1	A	718	TYR	CD2-CE2	-5.11	1.31	1.39
1	A	718	TYR	CD1-CE1	-5.09	1.31	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	ARG	N-CA-CB	-17.24	79.57	110.60
1	A	186	GLN	N-CA-CB	-15.15	83.34	110.60
1	A	367	LEU	N-CA-CB	-10.62	89.16	110.40
1	A	1080	ARG	N-CA-C	8.35	133.54	111.00
1	A	330	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	725	CYS	CA-CB-SG	-6.71	101.92	114.00
1	A	185	PRO	N-CA-C	6.32	128.54	112.10
1	A	327	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	576	LEU	CA-CB-CG	6.18	129.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	814	LEU	CB-CG-CD2	5.93	121.09	111.00
1	A	561	TRP	N-CA-C	5.85	126.80	111.00
1	A	327	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	1090	ASP	N-CA-CB	5.56	120.61	110.60
1	A	300	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	1074	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	1090	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	722	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	666	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	185	PRO	CB-CA-C	5.27	125.17	112.00
1	A	1078	THR	N-CA-C	-5.27	96.77	111.00
1	A	314	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	389	ILE	CG1-CB-CG2	-5.15	100.06	111.40
1	A	644	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	375	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	A	932	LEU	CB-CG-CD1	-5.06	102.41	111.00
1	A	712	ILE	CB-CA-C	-5.04	101.51	111.60
1	A	374	GLN	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8726	0	8706	701	0
2	B	116	0	124	55	0
All	All	8842	0	8830	743	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (743) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:HIS:NE2	1:A:623:LEU:HB2	1.39	1.35
1:A:597:GLU:HB2	1:A:664:HIS:NE2	1.47	1.30
2:B:47:VAL:O	2:B:51:LYS:HG3	1.39	1.23
1:A:927:MET:O	1:A:928:ARG:HD3	1.38	1.23
2:B:51:LYS:HA	2:B:54:GLU:CG	1.73	1.19
2:B:50:LEU:O	2:B:54:GLU:HG2	1.44	1.17
1:A:578:HIS:CD2	1:A:623:LEU:HB2	1.77	1.17
1:A:469:ILE:HD11	1:A:471:ILE:HG13	1.25	1.14
1:A:98:ILE:H	1:A:98:ILE:HD13	1.16	1.10
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.01	1.09
1:A:367:LEU:HD12	1:A:374:GLN:HG3	1.24	1.09
1:A:620:THR:HG23	1:A:621:GLY:H	1.20	1.07
2:B:51:LYS:HA	2:B:54:GLU:HG3	1.12	1.07
1:A:631:LEU:N	1:A:631:LEU:HD23	1.70	1.06
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.20	1.05
2:B:45:SER:HB2	2:B:47:VAL:HG22	1.33	1.05
2:B:49:TYR:O	2:B:53:ARG:HG3	1.55	1.05
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.34	1.04
1:A:410:LEU:HD12	1:A:680:CYS:SG	1.98	1.02
1:A:367:LEU:HD12	1:A:374:GLN:CG	1.89	1.02
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.42	1.01
1:A:578:HIS:NE2	1:A:623:LEU:CB	2.22	1.01
1:A:870:VAL:HG11	1:A:873:MET:CE	1.89	1.01
1:A:1014:MET:SD	1:A:1015:GLN:HG2	2.00	1.01
1:A:400:ALA:H	1:A:701:ILE:HD11	1.22	1.01
1:A:38:ARG:HD2	1:A:54:GLU:OE1	1.60	0.99
1:A:1033:VAL:HG11	2:B:56:ARG:HB2	1.45	0.99
1:A:578:HIS:CE1	1:A:623:LEU:HD12	1.96	0.98
1:A:665:LYS:O	1:A:666:LEU:HG	1.63	0.98
1:A:98:ILE:H	1:A:98:ILE:CD1	1.76	0.98
1:A:597:GLU:CB	1:A:664:HIS:NE2	2.25	0.98
2:B:51:LYS:CA	2:B:54:GLU:CG	2.41	0.97
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.80	0.96
1:A:597:GLU:HB2	1:A:664:HIS:CD2	2.00	0.96
1:A:616:LEU:HG	1:A:617:ASN:H	1.28	0.95
1:A:928:ARG:O	1:A:928:ARG:HG2	1.65	0.95
1:A:175:ALA:HB3	1:A:194:GLU:HG2	1.48	0.95
1:A:812:TYR:HD1	2:B:51:LYS:NZ	1.63	0.95
2:B:51:LYS:CA	2:B:54:GLU:HG2	1.98	0.94
2:B:56:ARG:NH1	2:B:57:LEU:HB2	1.83	0.94
1:A:24:THR:H	1:A:30:ASN:HD21	1.14	0.94
1:A:614:PHE:HE2	1:A:625:ASP:O	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:HG	1:A:645:SER:H	1.29	0.93
1:A:870:VAL:HG11	1:A:873:MET:HE1	1.46	0.93
1:A:812:TYR:HD1	2:B:51:LYS:HZ3	1.14	0.92
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.51	0.92
1:A:614:PHE:HD2	1:A:624:SER:HG	1.18	0.92
1:A:367:LEU:CD1	1:A:374:GLN:HG3	1.99	0.91
1:A:1125:THR:HG22	1:A:1126:ALA:N	1.85	0.90
1:A:1033:VAL:CG1	2:B:56:ARG:HB2	1.99	0.90
2:B:51:LYS:O	2:B:54:GLU:HB2	1.72	0.90
1:A:530:SER:HB3	1:A:574:PHE:HE1	1.36	0.90
2:B:57:LEU:HD23	2:B:57:LEU:O	1.72	0.90
1:A:1125:THR:CG2	1:A:1126:ALA:H	1.84	0.89
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.02	0.89
1:A:133:LEU:HB3	1:A:135:LEU:CD2	2.03	0.89
1:A:518:TYR:HD2	1:A:519:LEU:N	1.70	0.88
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.39	0.88
1:A:931:LEU:N	1:A:931:LEU:HD12	1.88	0.88
1:A:516:LEU:HD11	1:A:534:MET:SD	2.14	0.87
1:A:475:SER:HB2	1:A:490:TRP:O	1.74	0.87
1:A:978:GLN:HE21	1:A:995:VAL:HG21	1.38	0.87
1:A:1075:SER:OG	1:A:1084:PRO:HA	1.74	0.86
1:A:23:PHE:H	1:A:30:ASN:HD22	1.20	0.86
1:A:642:ARG:NH2	1:A:683:ASN:HB2	1.91	0.86
1:A:614:PHE:CE2	1:A:625:ASP:O	2.28	0.85
1:A:620:THR:HG23	1:A:621:GLY:N	1.91	0.84
1:A:11:LYS:HE2	1:A:38:ARG:HE	1.39	0.84
1:A:597:GLU:CB	1:A:664:HIS:CD2	2.61	0.83
1:A:469:ILE:CD1	1:A:471:ILE:HG13	2.07	0.82
1:A:399:HIS:HB2	1:A:701:ILE:HG12	1.62	0.81
1:A:1080:ARG:O	1:A:1080:ARG:HG3	1.78	0.81
1:A:382:PHE:H	1:A:720:SER:HB3	1.46	0.81
1:A:81:THR:HG22	1:A:83:LYS:H	1.45	0.81
1:A:98:ILE:HD13	1:A:98:ILE:N	1.97	0.80
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.62	0.80
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.63	0.80
2:B:45:SER:CB	2:B:47:VAL:HG22	2.12	0.80
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.46	0.79
1:A:928:ARG:CG	1:A:928:ARG:O	2.30	0.79
1:A:107:ASN:OD1	1:A:109:GLN:HG2	1.82	0.79
1:A:587:ILE:HB	1:A:588:PRO:HD2	1.63	0.79
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:CD1	1:A:98:ILE:N	2.42	0.78
1:A:731:GLN:O	1:A:796:GLN:HG2	1.84	0.78
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.67	0.78
1:A:342:GLU:O	1:A:343:GLN:HB3	1.83	0.78
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.18	0.78
1:A:1024:THR:CB	1:A:1041:THR:HG21	2.14	0.78
1:A:630:THR:HG21	1:A:1134:GLU:OE1	1.82	0.78
1:A:181:VAL:HG13	1:A:212:VAL:HG21	1.66	0.78
2:B:50:LEU:C	2:B:54:GLU:HG2	2.04	0.78
1:A:139:LEU:HD22	1:A:156:ASN:HB3	1.66	0.77
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.64	0.77
1:A:81:THR:CG2	1:A:83:LYS:H	1.97	0.77
1:A:24:THR:H	1:A:30:ASN:ND2	1.83	0.77
1:A:1090:ASP:HB2	1:A:1092:ASP:HB2	1.65	0.77
2:B:50:LEU:O	2:B:54:GLU:CG	2.29	0.77
1:A:578:HIS:NE2	1:A:623:LEU:CD1	2.47	0.77
1:A:561:TRP:O	1:A:564:ILE:HD12	1.85	0.77
1:A:1105:MET:SD	1:A:1130:ILE:HD12	2.25	0.77
1:A:623:LEU:HD23	1:A:623:LEU:C	2.04	0.76
1:A:854:SER:HB2	1:A:857:LYS:HG2	1.67	0.76
1:A:400:ALA:N	1:A:701:ILE:HD11	2.00	0.76
1:A:133:LEU:HB3	1:A:135:LEU:HD21	1.65	0.76
1:A:81:THR:HB	1:A:85:ASN:HB2	1.67	0.76
2:B:57:LEU:C	2:B:57:LEU:HD23	2.04	0.76
1:A:513:GLY:O	1:A:538:VAL:HG23	1.85	0.76
1:A:523:PRO:O	1:A:524:GLN:HB2	1.85	0.76
2:B:55:VAL:O	2:B:56:ARG:CB	2.34	0.76
1:A:388:ARG:HD3	1:A:714:THR:OG1	1.86	0.75
1:A:922:LEU:O	1:A:932:LEU:HD12	1.87	0.75
1:A:927:MET:O	1:A:928:ARG:CD	2.30	0.74
1:A:324:VAL:HG12	1:A:324:VAL:O	1.87	0.74
1:A:410:LEU:CD1	1:A:680:CYS:SG	2.75	0.74
1:A:68:ARG:NH1	1:A:74:LYS:HA	2.02	0.74
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.70	0.74
1:A:449:MET:O	1:A:479:VAL:HG21	1.86	0.74
1:A:812:TYR:CD1	2:B:51:LYS:NZ	2.53	0.74
1:A:11:LYS:HE2	1:A:38:ARG:NE	2.03	0.74
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.70	0.74
1:A:661:SER:HA	1:A:666:LEU:HA	1.70	0.74
1:A:484:LYS:O	1:A:485:ALA:HB2	1.87	0.74
1:A:617:ASN:HB3	1:A:620:THR:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:SER:OG	1:A:134:ARG:CZ	2.37	0.73
1:A:130:MET:HA	1:A:145:LEU:HD12	1.69	0.73
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.69	0.73
1:A:213:GLU:OE1	1:A:236:SER:HB3	1.89	0.73
1:A:507:GLN:NE2	1:A:552:LEU:HA	2.00	0.73
1:A:480:SER:HB2	1:A:484:LYS:H	1.52	0.72
1:A:418:ASN:HD22	1:A:419:ARG:H	1.37	0.72
1:A:870:VAL:CG1	1:A:873:MET:HE3	2.20	0.72
1:A:438:LEU:HD23	1:A:442:GLU:O	1.90	0.72
1:A:256:SER:HB3	1:A:275:ASP:OD2	1.90	0.72
1:A:400:ALA:H	1:A:701:ILE:CD1	2.00	0.72
1:A:701:ILE:HD13	1:A:701:ILE:N	2.05	0.72
1:A:22:HIS:CD2	1:A:28:ASP:O	2.43	0.71
1:A:364:VAL:HG22	1:A:375:LEU:CD1	2.19	0.71
1:A:591:ILE:HD12	1:A:604:CYS:HB2	1.71	0.71
1:A:687:TYR:O	1:A:690:SER:HB2	1.91	0.71
1:A:414:ARG:HA	1:A:422:TYR:HA	1.72	0.71
1:A:117:GLU:HA	1:A:117:GLU:OE1	1.89	0.71
1:A:427:LEU:HD13	1:A:429:PHE:HD2	1.55	0.71
1:A:641:PHE:HA	1:A:681:PRO:CG	2.18	0.71
1:A:312:GLU:HG3	1:A:327:ARG:HG3	1.72	0.70
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.72	0.70
1:A:927:MET:O	1:A:928:ARG:HB3	1.90	0.70
1:A:312:GLU:HG3	1:A:327:ARG:CG	2.21	0.70
1:A:16:ASN:ND2	1:A:35:LYS:O	2.23	0.70
1:A:37:THR:HG22	1:A:59:GLY:O	1.92	0.70
1:A:1033:VAL:HG11	2:B:56:ARG:CB	2.22	0.70
1:A:394:ILE:HD11	1:A:669:SER:HB2	1.74	0.70
1:A:620:THR:CG2	1:A:621:GLY:H	2.02	0.70
1:A:1078:THR:O	1:A:1079:GLU:C	2.30	0.69
1:A:366:ASP:HB3	1:A:372:GLN:O	1.92	0.69
1:A:654:ASP:HA	1:A:675:GLU:CG	2.21	0.69
1:A:835:MET:O	1:A:843:PRO:HB3	1.92	0.69
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.25	0.69
1:A:374:GLN:OE1	1:A:391:ARG:HG3	1.93	0.69
1:A:364:VAL:HG22	1:A:375:LEU:HD12	1.75	0.69
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.27	0.69
1:A:103:ARG:HB3	1:A:103:ARG:HH11	1.56	0.69
1:A:642:ARG:HH21	1:A:683:ASN:HB2	1.56	0.69
1:A:272:LEU:O	1:A:273:LEU:HD23	1.93	0.68
1:A:426:VAL:HG22	1:A:435:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:HH12	2:B:57:LEU:HB2	1.57	0.68
1:A:870:VAL:CG1	1:A:873:MET:CE	2.66	0.68
2:B:51:LYS:C	2:B:54:GLU:HG2	2.13	0.68
1:A:930:VAL:C	1:A:931:LEU:HD12	2.13	0.68
1:A:427:LEU:HD13	1:A:429:PHE:CD2	2.29	0.68
1:A:342:GLU:O	1:A:343:GLN:CB	2.41	0.68
1:A:874:VAL:HG22	1:A:875:GLU:N	2.08	0.68
1:A:691:LEU:O	1:A:701:ILE:HA	1.93	0.68
1:A:931:LEU:N	1:A:931:LEU:CD1	2.56	0.68
2:B:52:ASN:C	2:B:54:GLU:N	2.45	0.68
1:A:414:ARG:NH1	1:A:414:ARG:HG2	2.04	0.68
1:A:853:TYR:HA	1:A:857:LYS:O	1.94	0.68
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.29	0.68
1:A:969:GLU:O	1:A:971:ALA:N	2.26	0.68
1:A:355:ASN:OD1	1:A:357:GLY:N	2.27	0.68
1:A:197:LEU:H	1:A:197:LEU:HD23	1.58	0.67
1:A:905:HIS:HD2	1:A:908:ASN:HD21	1.43	0.67
1:A:518:TYR:C	1:A:518:TYR:HD2	1.97	0.67
1:A:642:ARG:NH2	1:A:683:ASN:CB	2.58	0.67
1:A:613:TYR:CZ	1:A:627:LYS:HB2	2.29	0.67
2:B:55:VAL:O	2:B:56:ARG:HB2	1.95	0.67
1:A:570:LYS:NZ	1:A:572:PRO:HD2	2.10	0.67
1:A:923:VAL:HA	1:A:931:LEU:O	1.95	0.67
1:A:1078:THR:OG1	1:A:1080:ARG:HG2	1.95	0.67
1:A:159:LEU:HD23	1:A:161:GLU:H	1.60	0.67
1:A:341:ASN:HB2	1:A:342:GLU:OE1	1.94	0.66
1:A:385:GLY:HA3	1:A:719:GLU:O	1.95	0.66
1:A:419:ARG:HD3	1:A:421:THR:OG1	1.94	0.66
1:A:644:LEU:CG	1:A:645:SER:H	2.07	0.66
1:A:539:ALA:HB3	1:A:559:GLY:O	1.96	0.66
1:A:561:TRP:O	1:A:564:ILE:CD1	2.43	0.66
1:A:81:THR:CG2	1:A:82:ALA:N	2.58	0.66
1:A:978:GLN:NE2	1:A:995:VAL:HG21	2.08	0.66
2:B:48:TYR:O	2:B:52:ASN:HB2	1.95	0.66
2:B:51:LYS:CA	2:B:54:GLU:HG3	2.03	0.66
1:A:602:LEU:HD23	1:A:614:PHE:HB2	1.78	0.65
1:A:1044:SER:OG	1:A:1047:TRP:HB2	1.95	0.65
1:A:427:LEU:O	1:A:427:LEU:HD12	1.96	0.65
2:B:51:LYS:C	2:B:54:GLU:CG	2.65	0.65
1:A:366:ASP:OD1	1:A:366:ASP:N	2.29	0.65
1:A:803:HIS:CD2	1:A:858:LEU:HB2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:PHE:O	1:A:934:ALA:HA	1.96	0.65
1:A:364:VAL:HG21	1:A:1010:GLY:HA3	1.79	0.65
1:A:1123:GLU:HG2	1:A:1124:ALA:H	1.62	0.65
1:A:382:PHE:N	1:A:720:SER:HB3	2.11	0.65
1:A:480:SER:OG	1:A:487:VAL:HG21	1.96	0.65
1:A:5:TYR:CE2	1:A:7:VAL:CG2	2.80	0.65
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.15	0.65
1:A:653:SER:HB3	1:A:655:ARG:H	1.62	0.65
1:A:578:HIS:NE2	1:A:623:LEU:CG	2.59	0.64
1:A:234:GLN:O	1:A:236:SER:N	2.30	0.64
1:A:695:ASN:OD1	1:A:698:THR:HB	1.97	0.64
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.79	0.64
1:A:1054:MET:HE1	1:A:1129:LEU:HD12	1.79	0.64
1:A:714:THR:HG22	1:A:715:VAL:N	2.13	0.64
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.32	0.64
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.13	0.64
1:A:530:SER:CB	1:A:574:PHE:HE1	2.10	0.64
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.30	0.64
1:A:928:ARG:NE	1:A:928:ARG:O	2.30	0.64
1:A:18:CYS:N	1:A:313:CYS:SG	2.71	0.64
1:A:133:LEU:HB3	1:A:135:LEU:HD22	1.77	0.64
1:A:305:LEU:HD13	1:A:336:LEU:HD22	1.79	0.64
1:A:578:HIS:CE1	1:A:623:LEU:HB2	2.28	0.64
1:A:920:PHE:HB3	1:A:935:TYR:HB3	1.78	0.64
1:A:1033:VAL:HG13	2:B:55:VAL:O	1.99	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.78	0.63
1:A:396:ILE:HD12	1:A:673:LEU:HD21	1.81	0.63
1:A:342:GLU:N	1:A:342:GLU:OE1	2.30	0.63
1:A:372:GLN:NE2	1:A:372:GLN:O	2.32	0.63
1:A:598:SER:N	1:A:664:HIS:NE2	2.46	0.63
1:A:234:GLN:HA	1:A:234:GLN:OE1	1.99	0.63
1:A:518:TYR:C	1:A:518:TYR:CD2	2.71	0.63
1:A:615:GLY:H	1:A:624:SER:CB	2.12	0.63
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.34	0.63
1:A:471:ILE:HG12	1:A:476:VAL:HB	1.79	0.63
1:A:241:ASN:O	1:A:242:GLY:C	2.37	0.63
1:A:24:THR:N	1:A:30:ASN:HD21	1.90	0.63
1:A:985:THR:HG21	1:A:989:ARG:HH21	1.63	0.63
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.79	0.62
1:A:520:GLN:NE2	1:A:529:ILE:HD11	2.14	0.62
1:A:659:ILE:HA	1:A:667:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLU:HB3	1:A:749:THR:HB	1.80	0.62
1:A:500:VAL:CG1	1:A:541:LEU:HD12	2.30	0.62
1:A:750:THR:O	1:A:751:ALA:CB	2.48	0.62
1:A:5:TYR:HE2	1:A:7:VAL:CG2	2.12	0.62
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.63	0.62
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.81	0.62
1:A:367:LEU:HB2	1:A:368:GLU:OE1	2.00	0.62
2:B:52:ASN:O	2:B:54:GLU:N	2.33	0.62
1:A:276:MET:SD	1:A:276:MET:O	2.58	0.61
1:A:615:GLY:H	1:A:624:SER:HB3	1.65	0.61
1:A:367:LEU:HD12	1:A:374:GLN:CD	2.20	0.61
1:A:368:GLU:N	1:A:368:GLU:OE1	2.30	0.61
1:A:81:THR:HG22	1:A:83:LYS:N	2.14	0.61
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.81	0.61
1:A:593:MET:HA	1:A:601:TYR:O	2.01	0.61
1:A:34:ALA:HB2	1:A:64:MET:CE	2.31	0.61
1:A:81:THR:HG23	1:A:82:ALA:N	2.15	0.61
1:A:518:TYR:CD2	1:A:519:LEU:N	2.61	0.61
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.04	0.60
1:A:750:THR:O	1:A:751:ALA:HB2	2.01	0.60
1:A:265:ASP:OD2	1:A:270:ARG:NE	2.33	0.60
1:A:484:LYS:O	1:A:484:LYS:HG3	2.00	0.60
1:A:921:ILE:C	1:A:922:LEU:HD12	2.21	0.60
1:A:1025:GLN:O	1:A:1041:THR:HG23	2.01	0.60
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.81	0.60
1:A:367:LEU:CD1	1:A:374:GLN:CG	2.71	0.60
1:A:642:ARG:HH22	1:A:683:ASN:CB	2.14	0.60
1:A:459:PHE:HE2	1:A:461:GLY:CA	2.15	0.60
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.84	0.60
1:A:1033:VAL:HG13	2:B:56:ARG:HB2	1.83	0.60
1:A:493:PRO:O	1:A:494:GLN:HG2	2.00	0.60
1:A:927:MET:O	1:A:928:ARG:CB	2.49	0.60
1:A:985:THR:HB	1:A:989:ARG:HE	1.67	0.60
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.02	0.59
1:A:480:SER:CB	1:A:483:PRO:HD2	2.32	0.59
1:A:623:LEU:HD23	1:A:624:SER:N	2.17	0.59
1:A:1109:VAL:HG12	1:A:1110:ALA:H	1.67	0.59
1:A:139:LEU:HD22	1:A:156:ASN:CB	2.31	0.59
1:A:396:ILE:CD1	1:A:673:LEU:HD21	2.32	0.59
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.35	0.59
1:A:492:GLU:OE1	1:A:494:GLN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LEU:CD2	1:A:623:LEU:C	2.71	0.59
2:B:55:VAL:HG23	2:B:56:ARG:N	2.18	0.59
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.75	0.59
1:A:107:ASN:OD1	1:A:109:GLN:CG	2.50	0.59
1:A:20:THR:HB	1:A:315:THR:HG21	1.84	0.59
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.38	0.59
1:A:1061:VAL:HG13	1:A:1104:LYS:HD2	1.84	0.59
1:A:49:LEU:O	1:A:51:PRO:HD3	2.02	0.59
1:A:516:LEU:CD2	1:A:538:VAL:HG21	2.32	0.59
1:A:874:VAL:CG2	1:A:875:GLU:N	2.66	0.59
1:A:883:SER:H	1:A:914:LEU:HD11	1.67	0.59
2:B:57:LEU:CD2	2:B:57:LEU:C	2.71	0.59
1:A:484:LYS:O	1:A:485:ALA:CB	2.51	0.59
1:A:490:TRP:CD1	1:A:519:LEU:HD13	2.37	0.59
1:A:625:ASP:O	1:A:626:ARG:HB2	2.02	0.59
1:A:609:GLY:HA2	1:A:632:GLY:O	2.03	0.58
1:A:705:ASP:O	1:A:706:GLU:O	2.21	0.58
1:A:936:LYS:O	1:A:938:MET:N	2.28	0.58
1:A:1127:ASP:HA	1:A:1130:ILE:HG22	1.86	0.58
1:A:226:PHE:HB3	1:A:297:LEU:HD11	1.85	0.58
1:A:288:GLU:OE1	1:A:298:LYS:HE3	2.04	0.58
1:A:844:LYS:HD3	1:A:844:LYS:H	1.69	0.58
1:A:23:PHE:N	1:A:30:ASN:HD22	1.95	0.58
1:A:429:PHE:O	1:A:431:GLY:N	2.35	0.58
1:A:327:ARG:O	1:A:358:PRO:HD3	2.03	0.58
1:A:763:SER:C	1:A:803:HIS:HE1	2.06	0.58
1:A:726:TYR:HB2	1:A:733:PHE:HE2	1.69	0.58
1:A:719:GLU:OE2	1:A:755:SER:HB3	2.03	0.58
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.86	0.57
1:A:679:MET:HA	1:A:692:ALA:O	2.03	0.57
1:A:617:ASN:CB	1:A:620:THR:HG22	2.34	0.57
1:A:609:GLY:CA	1:A:632:GLY:O	2.52	0.57
1:A:889:ARG:HG3	1:A:904:ASN:HB3	1.85	0.57
1:A:570:LYS:HZ3	1:A:572:PRO:HD2	1.68	0.57
1:A:713:ARG:NH1	1:A:799:PHE:CD1	2.71	0.57
1:A:220:ILE:HB	1:A:230:ILE:HB	1.86	0.57
1:A:614:PHE:CD2	1:A:624:SER:OG	2.57	0.57
1:A:256:SER:CB	1:A:277:GLU:HG2	2.34	0.57
1:A:378:CYS:HB3	1:A:721:PRO:CB	2.31	0.57
1:A:480:SER:HB2	1:A:483:PRO:HB2	1.87	0.57
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:VAL:HG13	1:A:752:LEU:HD21	1.86	0.57
1:A:467:GLN:HE22	1:A:524:GLN:HA	1.69	0.57
1:A:639:ARG:HG3	1:A:640:THR:N	2.20	0.57
1:A:1050:LEU:HD21	1:A:1129:LEU:HD11	1.85	0.57
1:A:250:PRO:HG2	1:A:253:ILE:HG12	1.86	0.56
1:A:741:GLU:HG2	1:A:751:ALA:N	2.20	0.56
1:A:881:LEU:HD21	1:A:922:LEU:CD2	2.35	0.56
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.36	0.56
1:A:936:LYS:C	1:A:938:MET:H	2.09	0.56
2:B:56:ARG:O	2:B:57:LEU:C	2.43	0.56
1:A:410:LEU:HD13	1:A:425:LEU:HD21	1.88	0.56
1:A:482:GLU:HB2	1:A:483:PRO:CD	2.35	0.56
1:A:707:ILE:O	1:A:708:GLN:O	2.24	0.56
2:B:52:ASN:C	2:B:54:GLU:H	2.07	0.56
1:A:138:GLY:O	1:A:159:LEU:N	2.39	0.56
1:A:235:GLU:HG2	1:A:254:LYS:NZ	2.20	0.56
1:A:616:LEU:CG	1:A:617:ASN:H	2.06	0.56
1:A:378:CYS:SG	1:A:724:ILE:HB	2.45	0.56
1:A:457:THR:HG22	1:A:459:PHE:H	1.70	0.56
1:A:1052:LEU:O	1:A:1052:LEU:HD23	2.06	0.56
1:A:340:SER:HB2	1:A:344:GLY:C	2.27	0.55
1:A:665:LYS:O	1:A:666:LEU:CG	2.47	0.55
1:A:836:VAL:HG11	2:B:47:VAL:HG21	1.88	0.55
1:A:1077:HIS:C	1:A:1077:HIS:CD2	2.80	0.55
1:A:460:CYS:O	1:A:461:GLY:O	2.24	0.55
1:A:520:GLN:CD	1:A:529:ILE:HD11	2.27	0.55
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.37	0.55
1:A:889:ARG:HD3	1:A:901:THR:HG23	1.89	0.55
1:A:22:HIS:HD2	1:A:28:ASP:O	1.88	0.55
1:A:558:ILE:O	1:A:566:ALA:HA	2.06	0.55
1:A:644:LEU:HG	1:A:645:SER:N	2.12	0.55
1:A:559:GLY:HA2	1:A:565:SER:O	2.06	0.55
1:A:23:PHE:H	1:A:30:ASN:ND2	1.97	0.55
1:A:556:CYS:SG	1:A:557:ALA:N	2.79	0.55
1:A:578:HIS:CG	1:A:579:LYS:N	2.75	0.55
1:A:658:VAL:HG11	1:A:660:TYR:CD1	2.41	0.55
1:A:690:SER:OG	1:A:701:ILE:HB	2.06	0.55
1:A:534:MET:O	1:A:535:GLU:C	2.45	0.54
1:A:660:TYR:CD1	1:A:707:ILE:HG23	2.43	0.54
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.41	0.54
1:A:564:ILE:HG22	1:A:564:ILE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:CD2	1:A:614:PHE:HB2	2.36	0.54
1:A:614:PHE:HD2	1:A:624:SER:OG	1.85	0.54
1:A:412:PRO:O	1:A:413:LEU:HB2	2.07	0.54
1:A:765:VAL:HG13	1:A:766:SER:O	2.07	0.54
1:A:318:ASP:HB3	1:A:319:ASN:ND2	2.23	0.54
1:A:34:ALA:HB2	1:A:64:MET:HE2	1.90	0.54
1:A:535:GLU:HB3	1:A:536:HIS:CD2	2.43	0.54
1:A:701:ILE:N	1:A:701:ILE:CD1	2.71	0.54
1:A:563:ASP:CG	1:A:565:SER:HB3	2.28	0.54
1:A:714:THR:CG2	1:A:715:VAL:N	2.70	0.54
1:A:719:GLU:OE2	1:A:755:SER:CB	2.56	0.54
1:A:917:LYS:O	1:A:919:ASP:N	2.41	0.54
1:A:171:TYR:CD1	1:A:223:PRO:HA	2.43	0.54
1:A:522:HIS:O	1:A:524:GLN:N	2.41	0.54
1:A:528:GLN:O	1:A:529:ILE:HG12	2.08	0.53
1:A:726:TYR:HB2	1:A:733:PHE:CE2	2.43	0.53
1:A:803:HIS:CD2	1:A:858:LEU:CB	2.91	0.53
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.43	0.53
1:A:226:PHE:N	1:A:226:PHE:CD1	2.76	0.53
1:A:414:ARG:NH1	1:A:422:TYR:CE2	2.76	0.53
1:A:817:VAL:HG22	1:A:830:ILE:HB	1.89	0.53
1:A:969:GLU:OE2	1:A:971:ALA:HB3	2.07	0.53
1:A:609:GLY:N	1:A:633:THR:O	2.41	0.53
1:A:658:VAL:CG1	1:A:659:ILE:N	2.69	0.53
1:A:982:ALA:O	1:A:985:THR:HG22	2.08	0.53
1:A:1006:VAL:O	1:A:1030:PHE:HA	2.08	0.53
1:A:141:LYS:HE2	1:A:156:ASN:HD21	1.72	0.53
1:A:617:ASN:CB	1:A:620:THR:CG2	2.87	0.53
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.91	0.53
1:A:68:ARG:HH11	1:A:74:LYS:HA	1.71	0.53
1:A:203:ASN:O	1:A:204:LYS:C	2.47	0.53
1:A:578:HIS:CE1	1:A:579:LYS:O	2.62	0.53
2:B:52:ASN:O	2:B:53:ARG:C	2.43	0.53
1:A:421:THR:HG22	1:A:683:ASN:O	2.07	0.53
1:A:500:VAL:HG12	1:A:541:LEU:HD12	1.91	0.53
1:A:928:ARG:HA	1:A:929:SER:HB2	1.91	0.52
1:A:969:GLU:OE1	1:A:973:ASN:HB2	2.09	0.52
1:A:135:LEU:N	1:A:135:LEU:HD22	2.23	0.52
1:A:424:THR:HA	1:A:436:LEU:O	2.08	0.52
1:A:826:ASN:ND2	1:A:852:GLN:NE2	2.58	0.52
1:A:335:LYS:HB2	1:A:350:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:OG1	1:A:297:LEU:N	2.40	0.52
1:A:691:LEU:HD12	1:A:704:ILE:HD11	1.91	0.52
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.92	0.52
1:A:277:GLU:HA	1:A:277:GLU:OE1	2.09	0.52
1:A:1041:THR:HG22	1:A:1042:SER:O	2.10	0.52
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.91	0.52
1:A:632:GLY:O	1:A:633:THR:C	2.48	0.52
1:A:679:MET:C	1:A:679:MET:SD	2.89	0.52
1:A:707:ILE:HG22	1:A:708:GLN:N	2.24	0.52
1:A:571:LEU:CB	1:A:572:PRO:HD3	2.40	0.52
1:A:877:ASN:C	1:A:879:LYS:H	2.13	0.52
1:A:997:LEU:HD22	1:A:1076:PHE:CD1	2.45	0.51
1:A:467:GLN:OE1	1:A:521:ILE:HG22	2.11	0.51
1:A:569:LEU:HG	1:A:576:LEU:HA	1.90	0.51
1:A:606:LEU:HB2	1:A:608:ASP:OD2	2.10	0.51
1:A:466:GLN:HB3	1:A:481:GLN:HB2	1.92	0.51
1:A:38:ARG:NH1	1:A:56:GLY:CA	2.74	0.51
1:A:697:SER:O	1:A:698:THR:OG1	2.24	0.51
1:A:654:ASP:HA	1:A:675:GLU:HG2	1.91	0.51
1:A:542:ASP:O	1:A:556:CYS:SG	2.68	0.51
1:A:546:LEU:HD11	1:A:593:MET:SD	2.50	0.51
1:A:698:THR:HG22	1:A:700:THR:HG23	1.90	0.51
1:A:839:GLU:HG2	1:A:840:GLU:H	1.76	0.51
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.93	0.51
1:A:355:ASN:OD1	1:A:357:GLY:CA	2.59	0.51
1:A:459:PHE:CE2	1:A:461:GLY:CA	2.94	0.51
1:A:394:ILE:CD1	1:A:669:SER:HB2	2.40	0.51
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.93	0.50
1:A:490:TRP:NE1	1:A:519:LEU:HD22	2.27	0.50
1:A:262:ASN:ND2	1:A:316:TYR:H	2.09	0.50
1:A:475:SER:CB	1:A:490:TRP:O	2.53	0.50
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.46	0.50
1:A:890:LEU:O	1:A:890:LEU:HG	2.10	0.50
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.47	0.50
1:A:391:ARG:HD2	1:A:392:ASN:O	2.11	0.50
1:A:457:THR:OG1	1:A:470:GLN:NE2	2.37	0.50
1:A:38:ARG:CD	1:A:54:GLU:OE1	2.49	0.50
1:A:682:LEU:O	1:A:683:ASN:HB2	2.12	0.50
1:A:688:PRO:O	1:A:689:ASP:C	2.50	0.50
1:A:633:THR:OG1	1:A:634:GLN:N	2.43	0.50
1:A:151:GLU:HB2	1:A:153:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:O	1:A:631:LEU:O	2.29	0.50
1:A:763:SER:HA	1:A:803:HIS:CE1	2.46	0.50
1:A:1033:VAL:CG1	2:B:56:ARG:CB	2.81	0.50
1:A:492:GLU:HG3	1:A:512:VAL:HG21	1.94	0.50
1:A:537:GLU:HB3	1:A:561:TRP:CD1	2.47	0.50
1:A:487:VAL:HG12	1:A:524:GLN:O	2.12	0.50
1:A:530:SER:HB3	1:A:574:PHE:CE1	2.28	0.50
1:A:1078:THR:O	1:A:1079:GLU:O	2.29	0.49
1:A:683:ASN:CG	1:A:683:ASN:O	2.49	0.49
1:A:355:ASN:OD1	1:A:357:GLY:HA2	2.12	0.49
1:A:929:SER:HB2	1:A:950:ASN:O	2.12	0.49
2:B:51:LYS:N	2:B:54:GLU:HG2	2.26	0.49
1:A:141:LYS:HE2	1:A:156:ASN:ND2	2.27	0.49
1:A:459:PHE:HE2	1:A:461:GLY:HA3	1.77	0.49
1:A:564:ILE:CD1	1:A:564:ILE:N	2.76	0.49
1:A:763:SER:CA	1:A:803:HIS:CE1	2.96	0.49
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.48	0.49
1:A:255:GLN:HB3	1:A:279:ARG:NH2	2.27	0.49
1:A:563:ASP:O	1:A:564:ILE:O	2.30	0.49
1:A:181:VAL:HG13	1:A:212:VAL:CG2	2.40	0.49
1:A:414:ARG:HH12	1:A:422:TYR:HE2	1.61	0.49
1:A:658:VAL:HG11	1:A:660:TYR:CE1	2.47	0.49
1:A:23:PHE:N	1:A:30:ASN:ND2	2.60	0.49
1:A:632:GLY:O	1:A:634:GLN:O	2.31	0.49
1:A:395:GLY:HA2	1:A:672:ASN:HB2	1.94	0.49
1:A:917:LYS:CG	1:A:959:ILE:HG21	2.43	0.49
1:A:616:LEU:HG	1:A:617:ASN:N	2.11	0.48
1:A:538:VAL:HA	1:A:560:LEU:HD22	1.95	0.48
1:A:926:LEU:O	1:A:953:TRP:HA	2.12	0.48
1:A:458:PHE:O	1:A:459:PHE:HB2	2.13	0.48
1:A:563:ASP:OD1	1:A:564:ILE:N	2.46	0.48
1:A:932:LEU:HA	1:A:932:LEU:HD12	1.57	0.48
1:A:1054:MET:O	1:A:1058:LEU:HB2	2.13	0.48
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.47	0.48
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.95	0.48
1:A:426:VAL:HB	1:A:460:CYS:SG	2.54	0.48
1:A:987:GLU:C	1:A:989:ARG:H	2.16	0.48
1:A:304:LEU:HD12	1:A:305:LEU:N	2.27	0.48
1:A:563:ASP:C	1:A:563:ASP:OD1	2.49	0.48
1:A:905:HIS:CD2	1:A:908:ASN:HD21	2.28	0.48
1:A:1041:THR:HG22	1:A:1042:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:O	1:A:77:LEU:HD12	2.13	0.48
1:A:305:LEU:CD1	1:A:336:LEU:HD22	2.43	0.48
1:A:368:GLU:O	1:A:369:ARG:HB3	2.13	0.48
1:A:5:TYR:OH	1:A:1091:GLY:HA3	2.13	0.48
1:A:598:SER:O	1:A:599:SER:HB2	2.13	0.48
1:A:23:PHE:CD1	1:A:66:LEU:HD21	2.49	0.48
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.79	0.48
1:A:927:MET:O	1:A:927:MET:HG3	2.14	0.48
1:A:125:ASP:OD2	1:A:128:CYS:N	2.47	0.47
1:A:123:ILE:HG13	1:A:169:PHE:CE1	2.49	0.47
1:A:563:ASP:O	1:A:564:ILE:C	2.53	0.47
1:A:762:SER:O	1:A:763:SER:HB3	2.14	0.47
1:A:936:LYS:C	1:A:938:MET:N	2.67	0.47
1:A:116:SER:OG	1:A:134:ARG:NE	2.47	0.47
1:A:24:THR:HB	1:A:30:ASN:HD21	1.78	0.47
1:A:449:MET:HG2	1:A:484:LYS:HD2	1.95	0.47
1:A:698:THR:CG2	1:A:700:THR:HG23	2.44	0.47
1:A:449:MET:CG	1:A:484:LYS:HD2	2.43	0.47
1:A:631:LEU:N	1:A:631:LEU:CD2	2.44	0.47
1:A:109:GLN:HB2	1:A:109:GLN:HE21	1.46	0.47
1:A:728:GLU:O	1:A:731:GLN:N	2.30	0.47
1:A:112:ILE:HD12	1:A:112:ILE:N	2.29	0.47
1:A:235:GLU:HB3	1:A:254:LYS:HB2	1.97	0.47
1:A:234:GLN:C	1:A:236:SER:H	2.18	0.47
1:A:24:THR:N	1:A:30:ASN:ND2	2.57	0.47
1:A:600:HIS:CE1	1:A:618:ILE:HG23	2.50	0.47
1:A:921:ILE:HA	1:A:933:LEU:O	2.15	0.47
1:A:1131:LYS:HG2	1:A:1131:LYS:O	2.15	0.47
1:A:414:ARG:HH11	1:A:414:ARG:CG	2.20	0.47
1:A:580:GLU:CG	1:A:582:LEU:HD23	2.44	0.47
1:A:642:ARG:HH22	1:A:683:ASN:ND2	2.13	0.47
1:A:697:SER:O	1:A:698:THR:CB	2.62	0.47
1:A:81:THR:HG23	1:A:82:ALA:H	1.77	0.47
1:A:1048:TYR:HE2	1:A:1052:LEU:HD12	1.75	0.47
1:A:263:ARG:HB2	1:A:271:TYR:HE2	1.78	0.47
1:A:763:SER:C	1:A:803:HIS:CE1	2.88	0.47
1:A:117:GLU:CA	1:A:117:GLU:OE1	2.61	0.47
1:A:530:SER:CB	1:A:574:PHE:CE1	2.95	0.47
1:A:690:SER:O	1:A:691:LEU:HD23	2.15	0.47
1:A:130:MET:CA	1:A:145:LEU:HD12	2.41	0.46
1:A:632:GLY:HA3	1:A:653:SER:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:TYR:CE2	1:A:861:VAL:HG11	2.50	0.46
1:A:938:MET:CG	1:A:939:GLU:H	2.28	0.46
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.96	0.46
1:A:500:VAL:HG11	1:A:541:LEU:HD12	1.95	0.46
1:A:881:LEU:HD21	1:A:922:LEU:HD23	1.97	0.46
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.29	0.46
1:A:6:VAL:HG21	1:A:998:PHE:CE2	2.50	0.46
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.97	0.46
1:A:682:LEU:HB3	1:A:690:SER:HB3	1.98	0.46
1:A:38:ARG:NH1	1:A:56:GLY:HA3	2.29	0.46
1:A:658:VAL:HG12	1:A:659:ILE:N	2.28	0.46
1:A:1057:ARG:HD2	1:A:1108:VAL:O	2.16	0.46
1:A:40:GLU:HG3	1:A:54:GLU:HG2	1.98	0.46
1:A:641:PHE:CD2	1:A:650:PHE:HB2	2.51	0.46
1:A:1097:PHE:O	1:A:1100:ILE:HB	2.15	0.46
1:A:459:PHE:CE2	1:A:461:GLY:N	2.84	0.46
1:A:580:GLU:HG3	1:A:582:LEU:HD23	1.98	0.46
1:A:80:LEU:HG	1:A:81:THR:O	2.15	0.46
1:A:881:LEU:CD2	1:A:922:LEU:CD2	2.93	0.46
2:B:56:ARG:HH11	2:B:57:LEU:H	1.64	0.46
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.98	0.46
1:A:133:LEU:CB	1:A:135:LEU:HD21	2.42	0.46
1:A:235:GLU:HG2	1:A:254:LYS:HZ3	1.80	0.46
1:A:341:ASN:O	1:A:342:GLU:C	2.54	0.46
1:A:874:VAL:CG2	1:A:875:GLU:H	2.28	0.46
1:A:961:ASP:O	1:A:963:ASP:N	2.49	0.46
1:A:250:PRO:O	1:A:251:PRO:C	2.53	0.46
1:A:67:PHE:HD1	1:A:128:CYS:SG	2.38	0.46
1:A:564:ILE:HG21	1:A:583:GLY:O	2.15	0.45
1:A:5:TYR:HE2	1:A:7:VAL:HG21	1.79	0.45
1:A:155:PHE:HB3	1:A:200:LYS:HE3	1.97	0.45
1:A:355:ASN:ND2	1:A:357:GLY:HA2	2.30	0.45
1:A:394:ILE:HD11	1:A:669:SER:CB	2.45	0.45
1:A:411:TRP:HB2	1:A:460:CYS:HB2	1.98	0.45
1:A:630:THR:C	1:A:631:LEU:O	2.54	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.69	0.45
1:A:732:CYS:HB2	1:A:794:ILE:O	2.15	0.45
1:A:148:ASP:HB2	1:A:149:ASN:H	1.47	0.45
1:A:167:VAL:O	1:A:168:LYS:HG2	2.16	0.45
1:A:355:ASN:CG	1:A:357:GLY:HA2	2.37	0.45
1:A:490:TRP:CE2	1:A:519:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:TYR:HB3	1:A:661:SER:H	1.60	0.45
1:A:978:GLN:HE21	1:A:995:VAL:CG2	2.21	0.45
1:A:414:ARG:NH1	1:A:422:TYR:HE2	2.14	0.45
1:A:877:ASN:C	1:A:879:LYS:N	2.70	0.45
1:A:520:GLN:O	1:A:526:LEU:HA	2.16	0.45
1:A:402:ILE:O	1:A:698:THR:HA	2.16	0.45
1:A:1081:LYS:HE3	1:A:1083:GLU:HG2	1.98	0.45
1:A:14:ALA:HB1	1:A:327:ARG:HB3	1.98	0.45
1:A:879:LYS:HD2	1:A:890:LEU:HD21	1.98	0.45
1:A:20:THR:HB	1:A:315:THR:CG2	2.47	0.45
1:A:1079:GLU:O	1:A:1081:LYS:N	2.50	0.44
1:A:226:PHE:N	1:A:226:PHE:HD1	2.14	0.44
1:A:282:MET:HG3	1:A:284:LEU:HG	1.99	0.44
2:B:45:SER:OG	2:B:48:TYR:CE2	2.69	0.44
1:A:1033:VAL:HG11	2:B:56:ARG:CG	2.47	0.44
1:A:226:PHE:H	1:A:226:PHE:HD1	1.65	0.44
1:A:597:GLU:HB3	1:A:664:HIS:CD2	2.51	0.44
1:A:742:VAL:O	1:A:749:THR:HG22	2.17	0.44
1:A:81:THR:CB	1:A:85:ASN:HB2	2.43	0.44
1:A:1090:ASP:N	1:A:1090:ASP:OD2	2.49	0.44
1:A:520:GLN:HB2	1:A:522:HIS:HD2	1.82	0.44
1:A:611:LEU:HD23	1:A:611:LEU:C	2.37	0.44
1:A:641:PHE:HB3	1:A:679:MET:CE	2.47	0.44
1:A:817:VAL:CG1	1:A:873:MET:HG3	2.48	0.44
1:A:939:GLU:CG	1:A:941:ASN:HB2	2.47	0.44
1:A:1074:ARG:HA	1:A:1074:ARG:HD3	1.70	0.44
1:A:587:ILE:HB	1:A:588:PRO:CD	2.43	0.44
1:A:934:ALA:HB2	1:A:945:ILE:CD1	2.47	0.44
1:A:1109:VAL:HG12	1:A:1110:ALA:N	2.31	0.44
1:A:609:GLY:HA3	1:A:632:GLY:O	2.17	0.44
1:A:1055:GLN:HE21	1:A:1055:GLN:HB3	1.52	0.44
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.99	0.44
1:A:826:ASN:ND2	1:A:852:GLN:HE22	2.15	0.44
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.99	0.44
1:A:958:GLU:HG3	1:A:959:ILE:N	2.33	0.44
1:A:462:ASN:HD22	1:A:462:ASN:HA	1.68	0.44
1:A:579:LYS:HE3	1:A:580:GLU:O	2.17	0.44
1:A:985:THR:CG2	1:A:989:ARG:HH21	2.31	0.44
2:B:54:GLU:HA	2:B:54:GLU:OE1	2.18	0.44
1:A:1109:VAL:HG21	1:A:1125:THR:O	2.17	0.44
1:A:35:LYS:HB2	1:A:38:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:VAL:HG22	1:A:787:GLU:H	1.83	0.44
1:A:1041:THR:CG2	1:A:1042:SER:N	2.80	0.44
1:A:108:VAL:HG11	1:A:143:ILE:HD11	1.99	0.44
1:A:411:TRP:CZ2	1:A:459:PHE:HA	2.53	0.44
1:A:482:GLU:CB	1:A:483:PRO:CD	2.96	0.44
1:A:591:ILE:HD11	1:A:602:LEU:HD11	2.00	0.43
1:A:67:PHE:HD1	1:A:128:CYS:HG	1.66	0.43
1:A:1129:LEU:C	1:A:1131:LYS:H	2.21	0.43
1:A:141:LYS:HD2	1:A:154:ALA:HB3	1.99	0.43
1:A:388:ARG:CD	1:A:714:THR:OG1	2.59	0.43
1:A:731:GLN:C	1:A:796:GLN:HG2	2.39	0.43
1:A:1127:ASP:CA	1:A:1130:ILE:HG22	2.47	0.43
1:A:241:ASN:OD1	1:A:242:GLY:N	2.51	0.43
1:A:948:ASP:OD2	1:A:994:GLU:HG2	2.19	0.43
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.53	0.43
1:A:629:VAL:HG11	1:A:668:PHE:HE2	1.83	0.43
1:A:809:GLN:O	1:A:810:ASN:HB2	2.19	0.43
1:A:451:PHE:HA	1:A:470:GLN:OE1	2.19	0.43
1:A:563:ASP:OD2	1:A:567:ARG:NH1	2.52	0.43
1:A:965:PHE:O	1:A:976:VAL:HA	2.18	0.43
1:A:1078:THR:O	1:A:1078:THR:OG1	2.31	0.43
1:A:159:LEU:HD22	1:A:161:GLU:O	2.18	0.43
1:A:192:THR:HB	1:A:205:GLY:HA3	2.01	0.43
1:A:398:GLU:O	1:A:398:GLU:HG3	2.19	0.43
1:A:407:ILE:HG21	1:A:410:LEU:HD23	2.00	0.43
1:A:117:GLU:O	1:A:118:THR:CB	2.66	0.43
1:A:520:GLN:HB2	1:A:522:HIS:CD2	2.54	0.43
1:A:836:VAL:CG1	2:B:47:VAL:HG21	2.48	0.43
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.01	0.43
1:A:570:LYS:HB2	1:A:575:GLU:HG2	2.01	0.43
1:A:617:ASN:HB2	1:A:621:GLY:H	1.83	0.43
1:A:836:VAL:CG1	2:B:48:TYR:CE2	3.01	0.43
2:B:56:ARG:HH11	2:B:57:LEU:N	2.17	0.43
1:A:324:VAL:CG1	1:A:324:VAL:O	2.58	0.42
1:A:450:GLY:HA2	1:A:477:ARG:NH2	2.34	0.42
1:A:459:PHE:CD2	1:A:460:CYS:N	2.87	0.42
1:A:538:VAL:CG1	1:A:558:ILE:HD11	2.49	0.42
1:A:679:MET:HB2	1:A:693:LEU:HG	2.00	0.42
1:A:932:LEU:HD22	1:A:965:PHE:CE1	2.54	0.42
1:A:171:TYR:CG	1:A:223:PRO:HA	2.54	0.42
1:A:701:ILE:HD13	1:A:701:ILE:H	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:LEU:O	1:A:933:LEU:HD12	2.18	0.42
1:A:140:PHE:HB2	1:A:159:LEU:HD12	2.02	0.42
1:A:546:LEU:HD22	1:A:600:HIS:ND1	2.33	0.42
1:A:644:LEU:CG	1:A:645:SER:N	2.79	0.42
1:A:39:LEU:HD11	1:A:64:MET:SD	2.59	0.42
2:B:47:VAL:HG23	2:B:48:TYR:N	2.33	0.42
1:A:1049:ASN:O	1:A:1050:LEU:C	2.58	0.42
1:A:320:GLY:HA3	1:A:335:LYS:HE3	2.00	0.42
1:A:459:PHE:CD2	1:A:461:GLY:N	2.83	0.42
1:A:118:THR:O	1:A:118:THR:HG22	2.20	0.42
1:A:815:SER:HB3	1:A:872:SER:HA	2.02	0.42
1:A:861:VAL:O	1:A:861:VAL:HG12	2.19	0.42
1:A:969:GLU:C	1:A:971:ALA:H	2.21	0.42
2:B:46:LEU:O	2:B:50:LEU:HG	2.18	0.42
1:A:2:SER:CB	1:A:995:VAL:HG23	2.50	0.42
1:A:504:ASN:ND2	1:A:545:PRO:HD3	2.34	0.42
1:A:616:LEU:CG	1:A:617:ASN:N	2.80	0.42
1:A:580:GLU:OE1	1:A:623:LEU:HD11	2.19	0.42
2:B:55:VAL:CG2	2:B:56:ARG:N	2.82	0.42
1:A:438:LEU:C	1:A:440:GLY:H	2.23	0.42
2:B:45:SER:OG	2:B:48:TYR:HE2	2.03	0.42
1:A:181:VAL:HA	1:A:189:HIS:O	2.20	0.42
1:A:611:LEU:HD23	1:A:612:PHE:N	2.35	0.42
1:A:639:ARG:CG	1:A:640:THR:N	2.83	0.42
1:A:808:LEU:HD23	1:A:808:LEU:HA	1.92	0.42
1:A:727:GLN:HB2	1:A:829:PHE:CE1	2.55	0.42
1:A:864:LYS:HD3	1:A:899:VAL:HG23	2.01	0.42
1:A:88:ILE:O	1:A:89:LEU:HD23	2.20	0.42
1:A:928:ARG:HA	1:A:929:SER:CB	2.48	0.42
2:B:51:LYS:O	2:B:54:GLU:CB	2.55	0.42
2:B:55:VAL:O	2:B:56:ARG:HB3	2.14	0.42
1:A:706:GLU:O	1:A:707:ILE:HG13	2.19	0.41
2:B:55:VAL:HG23	2:B:56:ARG:H	1.85	0.41
1:A:1102:ARG:O	1:A:1105:MET:HB3	2.20	0.41
1:A:80:LEU:HD23	1:A:120:ILE:HG21	2.03	0.41
1:A:367:LEU:CG	1:A:374:GLN:HG3	2.48	0.41
1:A:449:MET:O	1:A:479:VAL:CG2	2.62	0.41
1:A:980:ASP:HB3	1:A:988:GLU:O	2.20	0.41
1:A:413:LEU:H	1:A:422:TYR:HB3	1.85	0.41
1:A:620:THR:CG2	1:A:621:GLY:N	2.64	0.41
1:A:742:VAL:CG1	1:A:752:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:LEU:HD22	1:A:965:PHE:HE1	1.85	0.41
1:A:138:GLY:O	1:A:159:LEU:CB	2.69	0.41
1:A:19:VAL:HG12	1:A:32:LEU:HB2	2.03	0.41
1:A:396:ILE:HD12	1:A:673:LEU:HD11	2.02	0.41
1:A:555:LEU:HD23	1:A:555:LEU:H	1.85	0.41
2:B:47:VAL:C	2:B:49:TYR:H	2.21	0.41
1:A:361:ASP:OD2	1:A:362:MET:N	2.54	0.41
1:A:660:TYR:CE2	1:A:707:ILE:HG12	2.56	0.41
1:A:879:LYS:HB2	1:A:890:LEU:HD11	2.03	0.41
1:A:234:GLN:C	1:A:235:GLU:HG3	2.40	0.41
1:A:641:PHE:HB3	1:A:679:MET:HE3	2.03	0.41
1:A:686:GLY:O	1:A:687:TYR:CG	2.74	0.41
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.74	0.41
1:A:824:ASP:OD2	1:A:893:TRP:NE1	2.49	0.41
1:A:893:TRP:HA	1:A:893:TRP:CE3	2.55	0.41
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.83	0.41
1:A:600:HIS:CE1	1:A:618:ILE:CG2	3.03	0.41
1:A:660:TYR:CE1	1:A:707:ILE:HA	2.55	0.41
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.03	0.41
1:A:1100:ILE:O	1:A:1105:MET:CE	2.69	0.41
1:A:884:ILE:HD12	1:A:889:ARG:HB2	2.03	0.41
1:A:1039:LEU:HD12	1:A:1040:VAL:N	2.36	0.41
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.56	0.41
1:A:611:LEU:HD23	1:A:612:PHE:C	2.41	0.41
1:A:909:ILE:HG21	1:A:927:MET:HG2	2.03	0.41
1:A:912:LEU:HD23	1:A:912:LEU:HA	1.80	0.41
1:A:928:ARG:CD	1:A:928:ARG:O	2.68	0.41
1:A:340:SER:HB3	1:A:346:TYR:CZ	2.55	0.41
1:A:607:GLY:HA2	1:A:635:PRO:HB3	2.02	0.41
1:A:730:SER:HB2	1:A:732:CYS:SG	2.61	0.41
1:A:741:GLU:HG2	1:A:750:THR:C	2.41	0.41
1:A:879:LYS:CB	1:A:890:LEU:HD11	2.51	0.41
1:A:953:TRP:CD1	1:A:953:TRP:N	2.88	0.41
1:A:24:THR:HG22	1:A:28:ASP:OD2	2.21	0.40
1:A:767:SER:OG	1:A:768:SER:N	2.54	0.40
1:A:1024:THR:CG2	1:A:1041:THR:HG21	2.50	0.40
1:A:169:PHE:HA	1:A:177:THR:O	2.21	0.40
1:A:155:PHE:CB	1:A:200:LYS:HE3	2.52	0.40
1:A:1123:GLU:HG2	1:A:1124:ALA:N	2.32	0.40
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.86	0.40
1:A:38:ARG:NH1	1:A:56:GLY:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:TYR:CE1	1:A:796:GLN:NE2	2.89	0.40
1:A:410:LEU:HD22	1:A:425:LEU:HD21	2.04	0.40
1:A:630:THR:HG21	1:A:1134:GLU:CD	2.39	0.40
1:A:2:SER:HB3	1:A:995:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1106/1143 (97%)	869 (79%)	167 (15%)	70 (6%)	1	7
2	B	11/13 (85%)	7 (64%)	2 (18%)	2 (18%)	0	0
All	All	1117/1156 (97%)	876 (78%)	169 (15%)	72 (6%)	1	7

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	235	GLU
1	A	318	ASP
1	A	407	ILE
1	A	430	VAL
1	A	461	GLY
1	A	485	ALA
1	A	487	VAL
1	A	494	GLN
1	A	523	PRO
1	A	554	PRO
1	A	571	LEU
1	A	624	SER
1	A	631	LEU

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Mol	Chain	Res	Type
1	A	665	LYS
1	A	683	ASN
1	A	698	THR
1	A	706	GLU
1	A	707	ILE
1	A	708	GLN
1	A	751	ALA
1	A	768	SER
1	A	918	GLY
1	A	919	ASP
1	A	928	ARG
1	A	970	ASN
1	A	1079	GLU
1	A	1080	ARG
1	A	1110	ALA
2	B	56	ARG
1	A	118	THR
1	A	242	GLY
1	A	474	ALA
1	A	505	SER
1	A	517	TYR
1	A	524	GLN
1	A	529	ILE
1	A	626	ARG
1	A	729	VAL
1	A	801	VAL
1	A	802	LEU
1	A	808	LEU
1	A	860	THR
1	A	886	SER
1	A	962	ASP
1	A	149	ASN
1	A	291	MET
1	A	343	GLN
1	A	413	LEU
1	A	535	GLU
1	A	564	ILE
1	A	599	SER
1	A	662	SER
1	A	689	ASP
1	A	856	GLY
1	A	1107	GLU

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Mol	Chain	Res	Type
2	B	53	ARG
1	A	503	CYS
1	A	518	TYR
1	A	620	THR
1	A	666	LEU
1	A	862	ALA
1	A	1130	ILE
1	A	810	ASN
1	A	864	LYS
1	A	929	SER
1	A	224	GLU
1	A	259	VAL
1	A	629	VAL
1	A	406	GLY
1	A	513	GLY
1	A	493	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	977/1001 (98%)	814 (83%)	163 (17%)	2	11
2	B	13/13 (100%)	11 (85%)	2 (15%)	2	13
All	All	990/1014 (98%)	825 (83%)	165 (17%)	2	11

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	VAL
1	A	19	VAL
1	A	25	SER
1	A	27	GLU
1	A	28	ASP
1	A	32	LEU

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Mol	Chain	Res	Type
1	A	35	LYS
1	A	49	LEU
1	A	55	VAL
1	A	79	ILE
1	A	81	THR
1	A	96	GLU
1	A	97	SER
1	A	98	ILE
1	A	103	ARG
1	A	109	GLN
1	A	117	GLU
1	A	125	ASP
1	A	128	CYS
1	A	130	MET
1	A	135	LEU
1	A	141	LYS
1	A	145	LEU
1	A	147	ARG
1	A	148	ASP
1	A	162	LEU
1	A	168	LYS
1	A	186	GLN
1	A	192	THR
1	A	197	LEU
1	A	218	MET
1	A	224	GLU
1	A	226	PHE
1	A	234	GLN
1	A	235	GLU
1	A	255	GLN
1	A	259	VAL
1	A	283	LEU
1	A	286	GLU
1	A	298	LYS
1	A	300	LEU
1	A	301	ARG
1	A	309	SER
1	A	312	GLU
1	A	314	LEU
1	A	321	VAL
1	A	327	ARG
1	A	331	SER

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	334	VAL
1	A	360	VAL
1	A	366	ASP
1	A	372	GLN
1	A	374	GLN
1	A	383	LYS
1	A	390	ILE
1	A	396	ILE
1	A	401	SER
1	A	410	LEU
1	A	411	TRP
1	A	414	ARG
1	A	418	ASN
1	A	419	ARG
1	A	424	THR
1	A	430	VAL
1	A	439	ASN
1	A	447	GLU
1	A	449	MET
1	A	452	VAL
1	A	462	ASN
1	A	467	GLN
1	A	468	LEU
1	A	469	ILE
1	A	476	VAL
1	A	492	GLU
1	A	496	LYS
1	A	503	CYS
1	A	506	SER
1	A	507	GLN
1	A	518	TYR
1	A	519	LEU
1	A	520	GLN
1	A	521	ILE
1	A	526	LEU
1	A	529	ILE
1	A	534	MET
1	A	544	THR
1	A	555	LEU
1	A	562	THR
1	A	564	ILE

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Mol	Chain	Res	Type
1	A	567	ARG
1	A	570	LYS
1	A	582	LEU
1	A	587	ILE
1	A	589	ARG
1	A	602	LEU
1	A	603	LEU
1	A	618	ILE
1	A	619	GLU
1	A	629	VAL
1	A	630	THR
1	A	633	THR
1	A	639	ARG
1	A	653	SER
1	A	654	ASP
1	A	668	PHE
1	A	669	SER
1	A	679	MET
1	A	701	ILE
1	A	703	THR
1	A	705	ASP
1	A	706	GLU
1	A	708	GLN
1	A	729	VAL
1	A	730	SER
1	A	744	ASP
1	A	750	THR
1	A	766	SER
1	A	794	ILE
1	A	814	LEU
1	A	815	SER
1	A	817	VAL
1	A	823	LYS
1	A	844	LYS
1	A	855	ASP
1	A	857	LYS
1	A	858	LEU
1	A	885	ASN
1	A	886	SER
1	A	893	TRP
1	A	896	GLU
1	A	899	VAL

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Mol	Chain	Res	Type
1	A	900	ARG
1	A	904	ASN
1	A	914	LEU
1	A	916	THR
1	A	917	LYS
1	A	922	LEU
1	A	928	ARG
1	A	931	LEU
1	A	945	ILE
1	A	947	ARG
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	986	ASP
1	A	992	LEU
1	A	1000	LEU
1	A	1006	VAL
1	A	1014	MET
1	A	1015	GLN
1	A	1039	LEU
1	A	1045	GLU
1	A	1055	GLN
1	A	1063	LYS
1	A	1075	SER
1	A	1079	GLU
1	A	1080	ARG
1	A	1093	LEU
1	A	1100	ILE
1	A	1127	ASP
1	A	1135	GLU
2	B	45	SER
2	B	49	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	30	ASN
1	A	109	GLN
1	A	189	HIS
1	A	261	HIS
1	A	262	ASN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	319	ASN
1	A	372	GLN
1	A	399	HIS
1	A	418	ASN
1	A	456	GLN
1	A	462	ASN
1	A	504	ASN
1	A	520	GLN
1	A	522	HIS
1	A	617	ASN
1	A	677	ASN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	826	ASN
1	A	845	GLN
1	A	852	GLN
1	A	885	ASN
1	A	905	HIS
1	A	941	ASN
1	A	950	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1015	GLN
1	A	1055	GLN
1	A	1056	ASN
1	A	1077	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1114/1143 (97%)	-0.08	40 (3%) 42 17	18, 68, 160, 208	0
2	B	13/13 (100%)	0.40	2 (15%) 2 1	30, 31, 32, 47	0
All	All	1127/1156 (97%)	-0.07	42 (3%) 41 17	18, 67, 160, 208	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ASN	7.8
1	A	294	THR	7.5
1	A	291	MET	7.3
1	A	483	PRO	6.4
1	A	616	LEU	6.3
1	A	508	VAL	5.5
1	A	292	ASP	5.4
1	A	293	GLY	5.2
1	A	773	SER	4.5
1	A	621	GLY	4.3
1	A	289	GLU	4.2
1	A	519	LEU	4.2
1	A	503	CYS	3.8
1	A	772	SER	3.7
1	A	545	PRO	3.5
1	A	569	LEU	3.3
1	A	521	ILE	3.2
1	A	482	GLU	3.2
1	A	625	ASP	3.1
1	A	547	GLY	3.1
1	A	599	SER	3.0
1	A	447	GLU	3.0
1	A	295	VAL	2.9
1	A	660	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	505	SER	2.8
1	A	369	ARG	2.7
1	A	506	SER	2.7
1	A	507	GLN	2.6
1	A	571	LEU	2.5
1	A	619	GLU	2.5
1	A	504	ASN	2.4
1	A	1015	GLN	2.4
1	A	528	GLN	2.4
1	A	518	TYR	2.3
2	B	56	ARG	2.3
1	A	468	LEU	2.3
1	A	542	ASP	2.2
1	A	502	SER	2.2
1	A	290	GLN	2.2
1	A	444	GLU	2.1
1	A	661	SER	2.1
2	B	57	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.